



TITLE:

# Genomic Object Net: Towards Biopathway Modeling and Simulation (BIOINFORMATICS CENTER - Pathway Engineering)

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## Bioinformatics Center - Pathway Engineering -



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### Scope of Research

This laboratory develops research on computational knowledge discovery, e.g. inference of pathway information from gene expression profile data, and simulation system for cells and organisms through the biopathway simulation of gene regulatory networks, signaling pathways, metabolic pathways, and physical simulations, etc. With this approach, the functions of genes and systems of genes will be analyzed and predicted.

### Research Activities (Year 2001)

#### Presentations

Views: fundamental building blocks in the process of knowledge discovery, Bannai H, Tamada Y, Maruyama O, Miyano S, The 14th International FLAIRS Conference, Florida, 21-23 May.

Selecting informative genes for cancer classification using gene expression data, Akutsu, T, Miyano, S, IEEE-EURASIP Workshop on Non-linear Signal and Image Processing - NSIP-01, Baltimore, 1-3 June.

VML: a view modeling language for computational knowledge discovery, Bannai H (U Tokyo), Tamada Y (Tokai U), Maruyama O (Kyushu U), Miyano S, The Fourth International Conference on Discovery Science, Washington DC, 26-28 November.

Learning conformation rules, Maruyama O, Shoudai T, Furuichi E, Kuhara S, Miyano S, The Fourth International Conference on Discovery Science, Washington DC, 26-28 November.

XML documentation of biopathways and their simulations in Genomic Object Net, Matsuno H (Yamaguchi U), Doi A (Yamaguchi U), Hirata Y, Miyano S, The Twelfth

International Conference on Genome Informatics, Tokyo, 17-19 December.

Genomic Object Net: Hybrid Object Net Architecture and XML Visualization for Biopathway Simulation, Third Biopathway Consortium Meeting, Copenhagen, 19-20 July.

HypothesisCreator: concepts for accelerating the computational knowledge discovery process, Bannai H, Tamada Y, Maruyama O, Miyano S, The 18th Machine Intelligence Conference, York, England, 19-21 September.

#### Grants

Miyano S, Genome-Wide Analysis of Genes Related to Disease Susceptibility and Drug Responsiveness, Research for Future Programs by Japan Society for the Promotion of Science, 1 April 2000 - 31 March 2004.

Miyano S, Mathematical Foundations of Computational Knowledge Discovery from cDNA Microarray Data, Grant-in-Aid for Scientific Research (B)(1), 1 April 2000 - 31 March 2003.

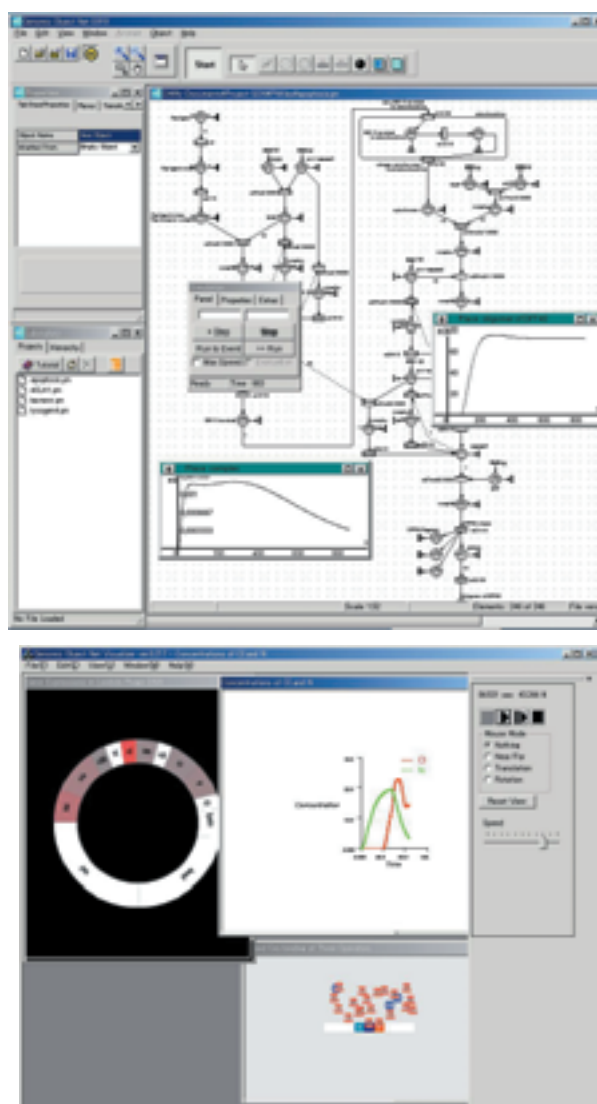
## Topics

### Genomic Object Net: Towards Biopathway Modeling and Simulation

Like in high-energy physics, if events in biological organisms could be simulated and predictions could be made on computers, such system would contribute to drug discovery and therapy in a drastically efficient way, and biology would be driven to a new era with a new methodology for discovery. This idea is not yet fully realized but some portions are being realized.

Biological knowledge in molecular and cellular biology has been typically represented as a series of natural language narratives together with schemes/pictures which would describe the processes of interactions and effects of various entities, e.g. molecules, stimuli, locations, etc. True understanding and interpretation of such knowledge often lie only in the human minds, i.e. experimental biologists.

We have been developing Genomic Object Net for modeling and simulating biopathways. Two key techniques are employed; hybrid functional Petri net (HFPN) for basic architecture, and XML for biopathway representation and simulation visualization. With Genomic Object Net, users can model biopathways as HFPNs based on their intuitive understanding and can result in confidence that the models designed with this software coincides with the understanding and knowledge in their minds. Our target pathways are structurally complex dynamic causal interactions and processes of various biological objects such as genomic DNA, mRNA, proteins, functional proteins, molecular transactions occurring at specific locations and time. For example, metabolic pathways, gene regulatory networks, and signal transduction cascades are counted as typical biopathways. With Genomic Object Net, we can observe *in silico* how these objects interact and behave quantitatively and qualitatively in biopathways. Genomic Object Net enables investigations which are usually impossible in experimental systems, such as searching for multiple small perturbations that produce large effects when they are combined. Differences between observed system behavior by simulation and observations in laboratory may suggest a change of model and will invoke new experiments for discovery. The large-scale modeling, such as the whole yeast biopathway modeling, is also feasible with the forthcoming version of this software if we combine various information from many difference sources, e.g. cDNA microarray data, protein interaction data, etc. The modeling process should go along with experimental activity in laboratory and Genomic Object Net will do so. The approach with such predictive simulations has obviously a big possibility to create a tremendous value in drug discovery and therapeutic development.



Genomic Object Net Snapshot

